3-Methyl-1-phenyl-1H-pyrazol-5-amine

1131-18-6 | DTXSID6044517

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 334 °C

Global applicability domain: Inside

Local applicability domain index: 3.26e-01

Confidence level: 5.20e-01

Nearest Neighbors from the Training Set

Image not found
3-Methyl-1-phenyl-1H-pyrazol-5-amine
Measured: 333
Predicted: 334

Image not found
4-Aminoazobenzene
Measured: 366
Predicted: 337

Image not found
2,4-Dinitroaniline
Measured: 334
Predicted: 330

Image not found
1,2,3-Benzotriazole
Measured: 350
Predicted: 294

Image not found
2,7,8,9-Tricyclazole
Measured: 275
Predicted: 290